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Mixture Model for Determination of Shock Equation of State

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14. ABSTRACT

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Mixture model for determination of shock equation of state

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Simple mixture models for the prediction of shock equations of state (Hugoniot) are a necessary tool for characterization of multiple composites. A mixture model for determining the shock equation of state of composite materials is presented. The model is completely flexible allowing for multiple (>2) components. Additionally, error propagation analysis for the two component mixture model has been accomplished. The model predicts the equation of state to 5%–15% of the experimental data, which is comparable to variations realized in meso-scale modeling of similar materials. [http://dx.doi.org/10.1063/1.3702873]

I. INTRODUCTION

As composites become increasingly used in applications where they are exposed to shock loading, a mixture model able to predict the shock equation of state based on the properties of the constituents is necessary.[1–13] However, models presented in the literature primarily account for only two component composites,[1–6] are restricted by geometry,[7] or require finite element software.[4–6,8] Bennett and Horie present a detailed mixture model for reactive powder composites, including calculating the volumetric mixture properties of the final compacted intermetallic material.[14] Current trends in mesoscale modeling have resulted in predictive capability for the properties of composites,[15–17] which require either high quality microstructures for the materials or the ability to artificially generate such microstructures. Given the differences in materials, particularly for polymer-based particulate composites consisting of hard particles in soft binders, the preparation of samples for microstructural analysis can be difficult.

There is very little discussion in the literature about the properties of the individual constituents, and how well they are known, affect the predicted properties of the composites. Often the models used are so complex as to prohibit the propagation of error from the constituent input terms.

This paper presents a non-reactive mixture model for fully dense composites, which can be implemented in a mathematical code, such as Matlab.[18] The model is flexible in the number of components that can be accommodate and is non-specific in the types of materials, e.g., polymer matrix composites and metallic alloys can both be accommodated. The error in the constituent properties has been propagated through the two-constituent model to determine the error bars for the calculated equation of state. Several two- and three-constituent composites are investigated with the model and compared with experimental data. The paper builds upon previous work which investigated the equation of state of epoxy-based particulate composites.[19]

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II. MIXTURE MODEL

A. Derivation of mixture model

In determining the nonreactive EOS for a multiphase mixture, mixture theory has been successfully applied to a variety of multiphase materials. A mixture shock Hugoniot is defined by determining the relationship of shock velocity to particle velocity, U_s and u_p, respectively.

Using jump state and characteristics theory,[1] the shock velocity is, by definition, $U_s = c_s + u_p$ and across a shock the change in density, for a two constituent mixture, is constrained by

$$\frac{\phi_1^0 \rho_1^0 + \phi_2^0 \rho_2^0}{\phi_1 \rho_1 + \phi_2 \rho_2} = 1 - \frac{u_p}{U_s}, \qquad (1)$$

where ϕ_k $(k = 1, 2)$ is the volume fraction, ρ_k $(k = 1, 2)$ is the true material density, and the 0 superscript corresponds to the undisturbed state. In the limit of homogeneous flow for a two constituent mixture, the mixture sound speed, c_s, is given by[20]

$$\frac{1}{c_s^2} = \frac{1}{(U_s - u_p)^2} = (\phi_1 \rho_1 + \phi_2 \rho_2)\left(\frac{\phi_1}{\rho_1 c_1^2} + \frac{\phi_2}{\rho_2 c_2^2}\right). \qquad (2)$$

For a saturated mixture,

$$\phi_1 + \phi_2 = 1 \qquad (3)$$

and the true density for each constituent is determined using the shock Hugoniot for the pure constituents,

$$\frac{\rho_k^0}{\rho_k} = 1 - \frac{u_p}{U_{s,k}} \qquad (4)$$

and

$$U_{s,k} = c_{0,k} + s_1 u_{p,k} + s_2 u_{p,k}^2. \qquad (5)$$

Therefore, a mixture shock velocity (corresponding to a specified particle velocity) is determined by combining Eqs. (1) and (2) and the resulting transcendental relationship

(for a specific volume fraction) is solved using a standard root solving method. The mixture quantities for pressure, P, and density are then defined by

$$P = P^0 + (\phi_1^0 \rho_1^0 + \phi_2^0 \rho_2^0) u_p U_s \tag{6}$$

and Eq. (1).

For a three constituent mixture, similar relationships hold and the procedure is applied first treating two constituents as a new "1 + 2" constituent given that $\phi_1^0 > 0$; hence, one defines a mixture-averaged density and sound speed, ρ_{12} and c_{12}. A normalized volume fraction is given by

$$\alpha = \frac{\phi_1}{\phi_1 + \phi_2} \tag{7}$$

and

$$\rho_{12} = \alpha \rho_1 + (1 - \alpha) \rho_2 \tag{8}$$

the mixture relationships of "1 + 2" phases are similar to Eqs. (2) and (4) rewritten in terms of the normalized volume fraction,

$$\frac{\rho_{12}^0}{\rho_{12}} = 1 - \frac{u_p}{U_{s,12}} = \frac{c_{12}}{u_p + c_{12}} \tag{9}$$

and

$$\frac{1}{c_{12}^2} = \frac{1}{(U_{s,12} - u_p)^2} = \left(\alpha \rho_1 + (1 - \alpha) \rho_2 \right) \left(\frac{\alpha}{\rho_1 c_1^2} + \frac{1 - \alpha}{\rho_2 c_2^2} \right). \tag{10}$$

Given the particle velocity, u_p, true densities for 1 and 2 are defined by their respective EOS in their pure state and α is solved combining Eqs. (9) and (10) and solving the resulting equation with a root solver.

Similar relationships are used for a new "1 + 3" constituent defining ρ_{13} and c_{13} by the following equations:

$$\beta = \frac{\phi_1}{\phi_1 + \phi_3}, \tag{11}$$

$$\rho_{13} = \beta \rho_1 + (1 - \beta) \rho_3, \tag{12}$$

$$\frac{\rho_{13}^0}{\rho_{13}} = 1 - \frac{u_p}{U_{s,13}} = \frac{c_{13}}{u_p + c_{13}}, \tag{13}$$

$$\frac{1}{c_{13}^2} = \frac{1}{(U_{s,13} - u_p)^2} = \left(\beta \rho_1 + (1 - \beta) \rho_3 \right) \left(\frac{\beta}{\rho_1 c_1^2} + \frac{1 - \beta}{\rho_3 c_3^2} \right), \tag{14}$$

and β is solved combining Eqs. (13) and (14), and the resulting equation is solved using a root solver.

Finally, for a three constituent system, the saturation constraint requires

$$\phi_1 + \phi_2 + \phi_3 = 1 \tag{15}$$

and with Eqs. (7) and (11), the shocked volume fractions are defined for a specified u_p,

$$\phi_1 = \frac{\alpha \beta}{\beta(1 - \alpha) + \alpha}, \tag{16a}$$

$$\phi_2 = \frac{\beta(1 - \alpha)}{\beta(1 - \alpha) + \alpha}, \tag{16b}$$

and

$$\phi_3 = \frac{\alpha(1 - \beta)}{\beta(1 - \alpha) + \alpha}. \tag{16c}$$

Conservation of mass across the jump state (shock) requires

$$\frac{\phi_1^0 \rho_1^0 + \phi_2^0 \rho_2^0 + \phi_3^0 \rho_3^0}{\phi_1 \rho_1 + \phi_2 \rho_2 + \phi_3 \rho_3} = 1 - \frac{u_p}{U_{s,123}}. \tag{17}$$

Hence, the wave speed for a three phase mixture, $U_{s,123}$, is defined as a function of particle velocity, u_p, producing the shock Hugoniot for a three phase system.

A similar procedure is applied to a multi-component mixture containing four or more constituents. In this general procedure, a reference component, subscripted by "1" such that $\phi_1^0 > 0$, and normalized variables are defined,

$$\alpha_j = \frac{\phi_j}{\phi_1 + \phi_j}, \tag{18}$$

$$\rho_{1j} = \alpha_j \rho_j + (1 - \alpha_j) \rho_1, \tag{19}$$

$$\frac{\rho_{1j}^0}{\rho_{1j}} = 1 - \frac{u_p}{U_{s,1j}} = \frac{c_{1j}}{u_p + c_{1j}}, \tag{20}$$

and

$$\frac{1}{c_{1j}^2} = \frac{1}{(U_{s,1j} - u_p)^2} = \left(\alpha_j \rho_j + (1 - \alpha_j) \rho_1 \right) \left(\frac{\alpha_j}{\rho_j c_j^2} + \frac{1 - \alpha_j}{\rho_1 c_1^2} \right). \tag{21}$$

The solution for all α_j (where $\alpha_j < 1$) can be determined upon specifying equations of state for each individual constituent and solving the sets of transcendental Equations (18)–(21). Since saturation implies that $\sum_{k=1}^{N} \phi_k = 1$, then

$$\phi_k = \frac{\alpha_k \phi_1}{1 - \alpha_k}, \quad \text{for } k = 2, N \tag{22}$$

hence,

$$\phi_1 = \frac{1}{\left(1 + \sum_{k=2}^{N} \frac{\alpha_k}{1 - \alpha_k} \right)} \tag{23a}$$

and

$$\phi_j = \frac{\alpha_j}{(1 - \alpha_j) \left(1 + \sum_{k=2}^{N} \frac{\alpha_k}{1 - \alpha_k} \right)} \tag{23b}$$

and the overall density change is then related to the mixture wave speed to define a mixture equation of state (i.e., shock Hugoniot) according to

$$\frac{\sum_{k=1}^{N} \phi_k^0 \rho_k^0}{\sum_{k=1}^{N} \phi_k \rho_k} = 1 - \frac{u_p}{U_{s,mix}}. \qquad (24)$$

B. Uncertainty analysis in mixture relationships

Along the Hugoniot, the mixture pressure, P, is related to the average particle velocity, u_p, and the mixture wave speed, U_s, by

$$P = \rho_0^{mix} u_p U_s, \qquad (25)$$

where ρ_0^{mix} is the undisturbed density. At a fixed particle velocity, it is readily seen that

$$\frac{\Delta P}{P} = \frac{\Delta U_s}{U_s} \qquad (26)$$

or the uncertainty associated with estimating pressure is directly related to the uncertainty in the mixture wave speed. Hence, the variations of mixture wave speed are assessed with regard to uncertainties of the individual constituents of the mixture.

For a two component mixture, consider

$$U_s = f(\rho_1^0, \rho_2^0, \phi_1^0, \phi_1, U_{s1}, U_{s2}) \qquad (27)$$

at conditions of fixed u_p. Following Ref. 21, the appropriate relationship for the uncertainty of mixture wave speed, dU_s, in terms of the uncertainties of variables in Eq. (27) is

$$dU_s = \left[\left(\frac{\partial U_s}{\partial \rho_1^0} d\rho_1^0 \right)^2 + \left(\frac{\partial U_s}{\partial \rho_2^0} d\rho_2^0 \right)^2 + \left(\frac{\partial U_s}{\partial \phi_1^0} d\phi_1^0 \right)^2 \right.$$
$$\left. + \left(\frac{\partial U_s}{\partial \phi_1} d\phi_1 \right)^2 + \left(\frac{\partial U_s}{\partial U_{s1}} dU_{s1} \right)^2 + \left(\frac{\partial U_s}{\partial U_{s2}} dU_{s2} \right)^2 \right]^{1/2}. \qquad (28)$$

The function for U_s is defined by the relationship for the mixture wave speed, i.e., Eq. (2), which, knowing that

$$\frac{\rho}{\rho_0} = \frac{U_s}{U_s - u_p}, \qquad (29)$$

can be rearranged as

$$\frac{1}{U_s(U_s - u_p)} = \rho_0^{mix} \left\{ \frac{\phi_1}{\rho_1^0 U_{s1}(U_{s1} - u_p)} + \frac{1 - \phi_1}{\rho_2^0 U_{s2}(U_{s2} - u_p)} \right\}. \qquad (30)$$

Partial differentiation of Eq. (30) in terms of each of the variables in Eq. (28) yields

$$dU_s = \left\{ (a_1 d\rho_1^0)^2 + (a_2 d\rho_2^0)^2 + (a_3 dU_{s1})^2 \right.$$
$$\left. + (a_4 dU_{s2})^2 + (a_2 d\phi_1^0)^2 + (a_6 d\phi_1)^2 \right\}^{1/2}, \qquad (31a)$$

where

$$a_1 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} \left(\frac{-(1 - \phi_1^0)\rho_2^0 \phi_1}{(\rho_1^0)^2 U_{s1}(U_{s1} - u_p)} + \frac{\phi_1^0(1 - \phi_1)}{\rho_2^0 U_{s2}(U_{s2} - u_p)} \right), \qquad (31b)$$

$$a_2 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} \left(\frac{(1 - \phi_1^0)\phi_1}{\rho_1^0 U_{s1}(U_{s1} - u_p)} - \frac{\phi_1^0 \rho_1^0(1 - \phi_1)}{(\rho_2^0)^2 U_{s2}(U_{s2} - u_p)} \right), \qquad (31c)$$

$$a_3 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} \left(\frac{\phi_1 \rho_0}{\rho_1^0} \right) \left(\frac{2U_{s1} - u_p}{(U_{s1}^2 - U_{s1} u_p)^2} \right), \qquad (31d)$$

$$a_4 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} \left(\frac{(1 - \phi_1)\rho_0}{\rho_2^0} \right) \left(\frac{2U_{s2} - u_p}{(U_{s2}^2 - U_{s2} u_p)^2} \right), \qquad (31e)$$

$$a_5 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} (\rho_1^0 - \rho_2^0)$$
$$\times \left(\frac{\phi_1}{\rho_1^0 U_{s1}(U_{s1} - u_p)} + \frac{1 - \phi_1}{\rho_2^0 U_{s2}(U_{s2} - u_p)} \right), \qquad (31f)$$

$$a_6 = \frac{(U_s^2 - U_s u_p)^2}{u_p - 2U_s} \rho_0 \left(\frac{1}{\rho_1^0 U_{s1}(U_{s1} - u_p)} - \frac{1}{\rho_2^0 U_{s2}(U_{s2} - u_p)} \right). \qquad (31g)$$

All of the terms in Eq. (31a) are known, except for the error in the volume fraction at pressure, $d\phi_1$, since the volume fraction at pressure is a derived quantity. However, this error can be determined by differentiating Eq. (1),

$$d\phi_1 = \left\{ (b_1 dU_s)^2 + (b_2 d\phi_1^0)^2 + (b_3 d\rho_1^0)^2 + (b_4 d\rho_2^0)^2 \right.$$
$$\left. + (b_5 dU_{s1})^2 + (b_6 dU_{s2})^2 \right\}^{1/2}. \qquad (32a)$$

where

$$b_1 = \frac{-u_p}{(U_s - u_p)^2 \delta_{p12}}, \qquad (32b)$$

$$b_2 = \frac{(\rho_1^0 - \rho_2^0)U_s}{(U_s - u_p)\rho_0 \delta_{p12}}, \qquad (32c)$$

$$b_3 = \frac{\left(\frac{\rho_0 U_s}{U_s - u_p} - \frac{\rho_2^0 U_{s2}}{U_{s2} - u_p} \right) \left(\frac{U_{s1}}{(U_{s1} - u_p)} \right)}{-(\rho_1^0)^2}, \qquad (32d)$$

$$b_4 = \frac{\left(\frac{\rho_0 U_s}{(U_s - u_p)} - \frac{\rho_2^0 U_{s1}}{(U_{s1} - u_p)} \right) \left(\frac{U_{s2}}{(U_{s2} - u_p)} \right)}{-(\delta_{p12}\rho_0)^2}, \qquad (32e)$$

$$b_5 = \left(\frac{-\rho_1^0 u_p}{(U_{s1} - u_p)^2} \right) \frac{\left(\frac{\rho_0 U_s}{(U_s - u_p)} - \frac{\rho_2^0 U_{s2}}{(U_{s2} - u_p)} \right)}{-(\delta_{p12}\rho_0)^2}, \qquad (32f)$$

TABLE I. Constituent and composite parameters for uranium with 13.4 wt. % rhodium.

Material	ρ_0 (g/cm^3)	C_0 (km/s)	S	ϕ^0	$d\rho_0$	$d\phi^0$	dU_s	Refs.
U	18.93	2.51	1.51	0.735	0.05	0.001	0.061	22
Rh	12.429	4.79	1.36	0.265	0.05		0.058	22
U-13.4 wt. % Rh	17.20	2.74	1.49					22

$$b_6 = \left(\frac{-\rho_2^0 u_p}{(U_{s2} - u_p)^2} \right) \frac{\left(\frac{\rho_0 U_s}{(U_s - u_p)} - \frac{\rho_1^0 U_{s1}}{(U_{s1} - u_p)} \right)}{-(\delta_{p12}\rho_0)^2}, \quad (32g)$$

and

$$\delta_{p12} = \frac{1}{\rho_0} \left[\frac{\rho_1^0 U_{s1}}{(U_{s1} - u_p)} - \frac{\rho_2^0 U_{s2}}{(U_{s2} - u_p)} \right]. \quad (33)$$

Equation (30) can be substituted into Eq. (31a) and rearranged to solve for dU_s,

$$dU_s = \left\{ \left(\frac{1}{1 - a_6^2 b_1^2} \right) \left[(a_1^2 + a_6^2 b_3^2)(d\rho_1^0)^2 + (a_2^2 + a_6^2 b_4^2)(d\rho_2^0)^2 \right. \right.$$
$$+ (a_3^2 + a_6^2 b_{55}^2)(dU_{s1})^2 + (a_4^2 + a_6^2 b_6^2)(dU_{s2})^2$$
$$\left. \left. + (a_5^2 + a_6^2 b_2^2)(d\phi_1^0)^2 \right] \right\}^{1/2}. \quad (34)$$

The error propagation for systems containing three or more components is increasingly complex and is not considered in this paper.

III. COMPARISON WITH EXPERIMENTAL DATA

A. Two-constituent composites

1. Uranium-rhodium composite

Uranium-rhodium (U-13.4 wt. % Rh) was chosen as a model metal-metal composite.[22] The properties for each constituent used in the model are given in Table I. The bulk sound speed, C_o, and S were determined from linear least squares fit to the available data[22] as shown in Figs. 1(a) and 1(b) for uranium and rhodium, respectively. The deviation from these linear fits, dU_s, were also determined and are shown in Fig. 1 and Table I.

The predicted Hugoniot relationship for U-13.4 wt. % Rh was determined from the mixture model for two constituents presented above. It can be seen from Fig. 2(a) that the model slightly overpredicts the experimental data, with an average deviation, dU_s/U_s of 0.05, shown in Fig. 2(b). The linear fits for uranium and rhodium are shown for comparison.

The propagated error associated with the input parameters to the mixture model was determined from Eq. (34) and is shown as the dashed lines bracketing the solid line in Fig. 2(a). The error in density was determined from the differences in the reported density values for uranium, and the same error was used for the density in rhodium. The density of the composite determined from the mixture model calculation agrees with that reported for the composite.[22] In order to determine the error in the input volume fraction, it was assumed that there was +/− 1 unit error in the last reported significant figure. The error in the shock velocity for both constituents is the dU_s values shown in Figs. 1(c) and 1(d).
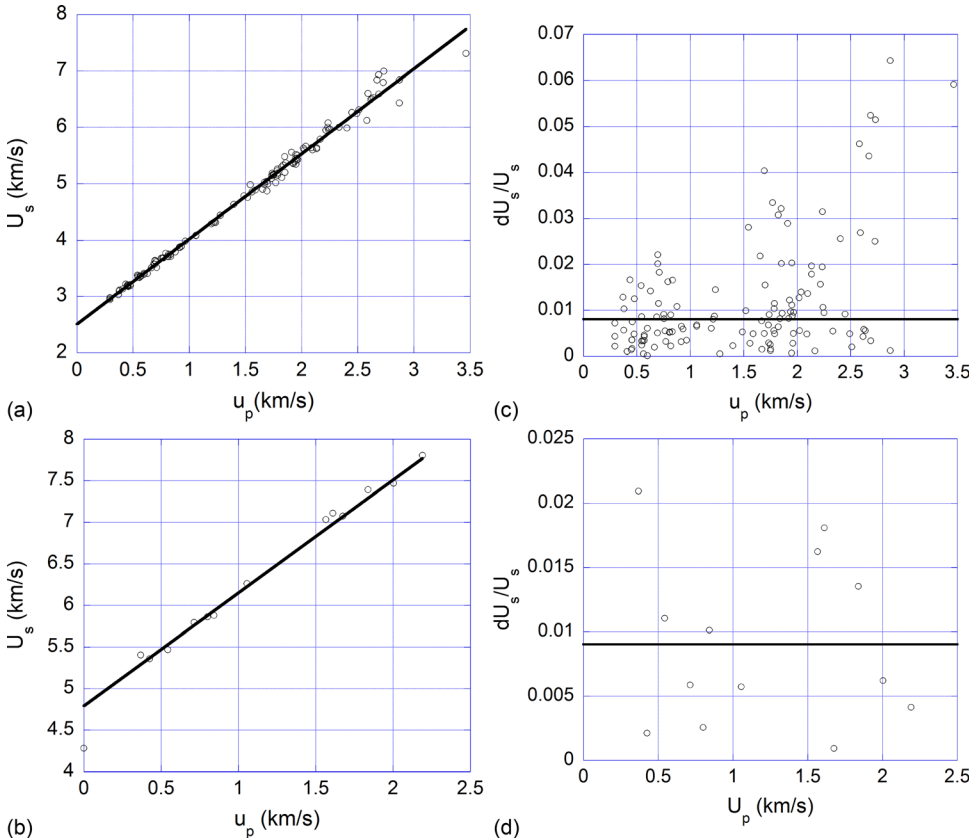

FIG. 1. Particle velocity vs shock velocity for (a) uranium and (b) rhodium, where the circles are the experimental data from Ref. 20 and the solid line is a linear fit to these experimental data, and dU_s/U_s for (c) uranium and (d) rhodium.
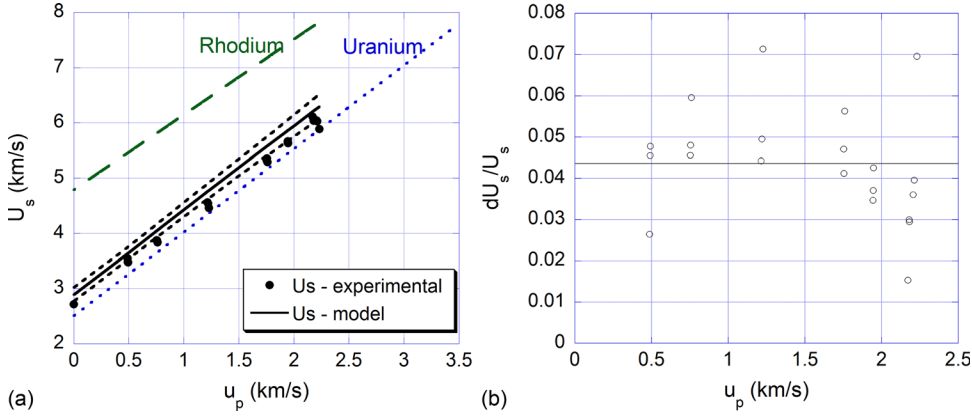
FIG. 2. (a) Particle velocity vs shock velocity and (b) dU_s/U_s for uranium, 13.4 wt.% rhodium experimental data (Ref. 20) compared with the mixture model calculation. The dashed lines on either side of the solid line in (a) indicated the error bars for the model calculation.

The experimental data[22] seem to lie on or around the lower error bar for this composite.

2. Epoxy-aluminum and epoxy-alumina composites

Two epoxy-based two-phase particulate composites were considered: Al$_2$O$_3$-57 vol % epoxy[23–26] and Al-55 vol % epoxy.[27] The former material has been extensively studied in the literature and the experimental data points used are combined from multiple references.[23–26] The latter material had a limited number of experimental Hugoniot points available, but a comparison between a polymer-based composite containing a metal powder and one containing an oxide powder should be useful.

The properties of the constituent materials are presented in Table II (Refs. 22–32) and Fig. 3. The epoxy used in this study appears to undergo a phase change around $u_p = 2.84$ km/s, Fig. 3(a). In order accommodate this phase change as well as a downturn in U_s at low values of u_p, a piecewise fit to the $U_s - u_p$ data for epoxy were used and is listed in Table III. In order to propagate the error from the input parameters through the model to determine the error bars in the output, the variations in the input parameters must be known. The variation in shock velocity, dU_s, was determined from the difference between the experimental data points and the linear least squares fit to the $U_s - u_p$ data. This variation is presented graphically in Figs. 3(d)–3(f) and

tabulated in Table II. Alumina deviates significantly from a linear $U_s - u_p$ fit in the low pressure regime. Here the average dU_s, used in propagating the error for the mixture, may not be representative. The variation in density for each of the materials was determined from either the variation in reported densities in the literature or assuming a variation of $+/-1$ unit in the last reported significant figure.

The model prediction along with the experimental data for Al$_2$O$_3$-57 vol % epoxy is presented in Fig. 4(a) and for Al-55 vol % epoxy in Fig. 4(c), along with the linear fits for the constituents. The model prediction underpredicts the data for Al$_2$O$_3$-57 vol % epoxy by approximately 14% (Fig. 4(b)). The prediction for Al-55 vol % epoxy is better at approximately 5%; however, there exists limited data points available to compare to the model predictions.

B. Multi-component composites

1. 304 stainless steel

304 stainless steel was chosen as a representative three constituent composite, with the primary constituents, 74% Fe, 18% Ni, and 8% Cr,[33] considered in this study. The phase change in iron was neglected in the model, although it could be incorporated in the same method as the epoxy above. The properties for each constituent used in the model are given in Table IV. The bulk sound speed, C_o, and S were

TABLE II. Constituent and composite parameters for epoxy-aluminum and epoxy-alumina materials.

Material	ρ_0 (g/cm^3)	C_0 (km/s)	S	ϕ^0_{epoxy}	$d\rho_0$	$d\phi^0$	dU_s	Ref.
Epoxy	1.134–1.194 [a]				0.03		0.09	28–32
Aluminum	2.712	5.33	1.38		0.001		0.06	22
Alumina	3.976	8.14	1.28		0.007		0.24	22
Epoxy-Al$_2$O$_3$ (300/100/20)	2.37	2.93	1.94	0.58		0.01		23
Epoxy-Al$_2$O$_3$ (Al2)	2.377	2.88	1.99	0.57		0.01		24
Epoxy-Al$_2$O$_3$ (Al3)	2.389			0.57		0.01		24
Epoxy-Al$_2$O$_3$ (Al4)	2.391			0.57		0.01		24
Epoxy-Al$_2$O$_3$ (fully loaded)	2.28	2.93	1.63	0.57		0.01		25
Epoxy-Al$_2$O$_3$ (F1)	2.376	2.76	2.26			0.01		26
Epoxy-Al$_2$O$_3$ (F2)	2.429	2.02	2.26			0.01		26
Epoxy-Al (Epoxy-45X81)	1.875			0.55		0.01		27

[a]Dependent on resin and curing agent.

TABLE III. Input parameters for mixture and mesoscale models.

Parameter	Epoxy Phase I	Epoxy Phase II	Epoxy Phase III	Epoxy Phase IV
u_p range	0–0.4	0.4–2.81	2.81–3.1	3.1–5.2
C_0 (km/s)	2.263	2.67	7.17	2.88
S	3.4704	1.55	0.01	1.35
S_2	−0.3947			

determined from linear least squares fits for Ni and Cr (Ref. 22) and used as reported in Ref. 34 for Fe.

The predicted Hugoniot relationship for 304 stainless steel was determined from the mixture model for three constituents presented above. It can be seen from Fig. 5 that the model slightly underpredicts the experimental data, with an average deviation, dU_s/U_s of 0.05, shown in Fig. 5(b). The linear fits for iron, nickel, and chromium are shown for comparison. The model may be improved by the addition of the minor components in 304 stainless steel and inclusion of the
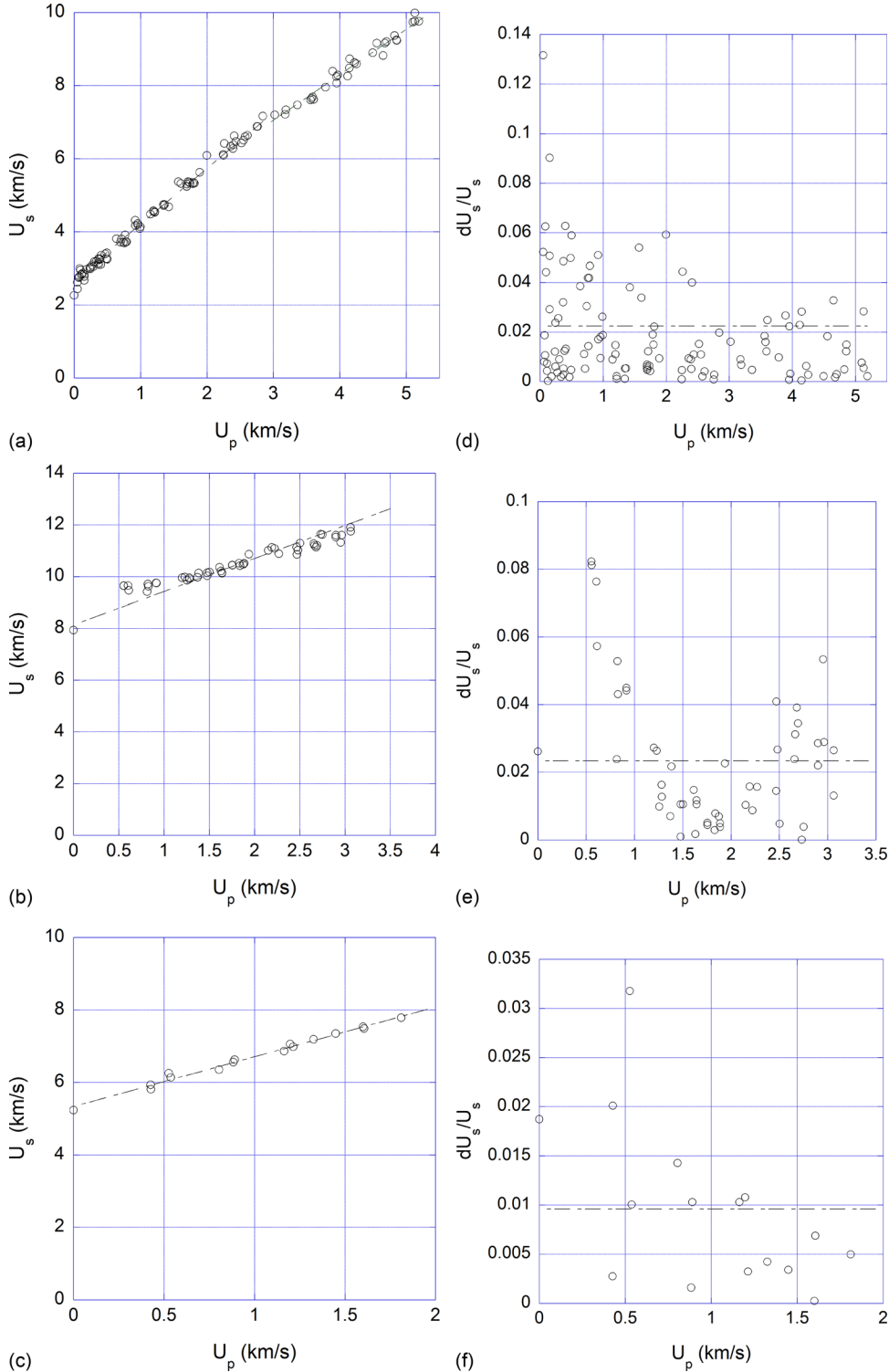

FIG. 3. Particle velocity vs shock velocity for (a) epoxy, (b) alumina, and (c) aluminum, where the circles are the experimental data from Refs. 20, 26–30, and the solid line is a linear least squares fit to this experimental data, and dU_s/U_s for (d) epoxy, (e) alumina, and (f) aluminum.
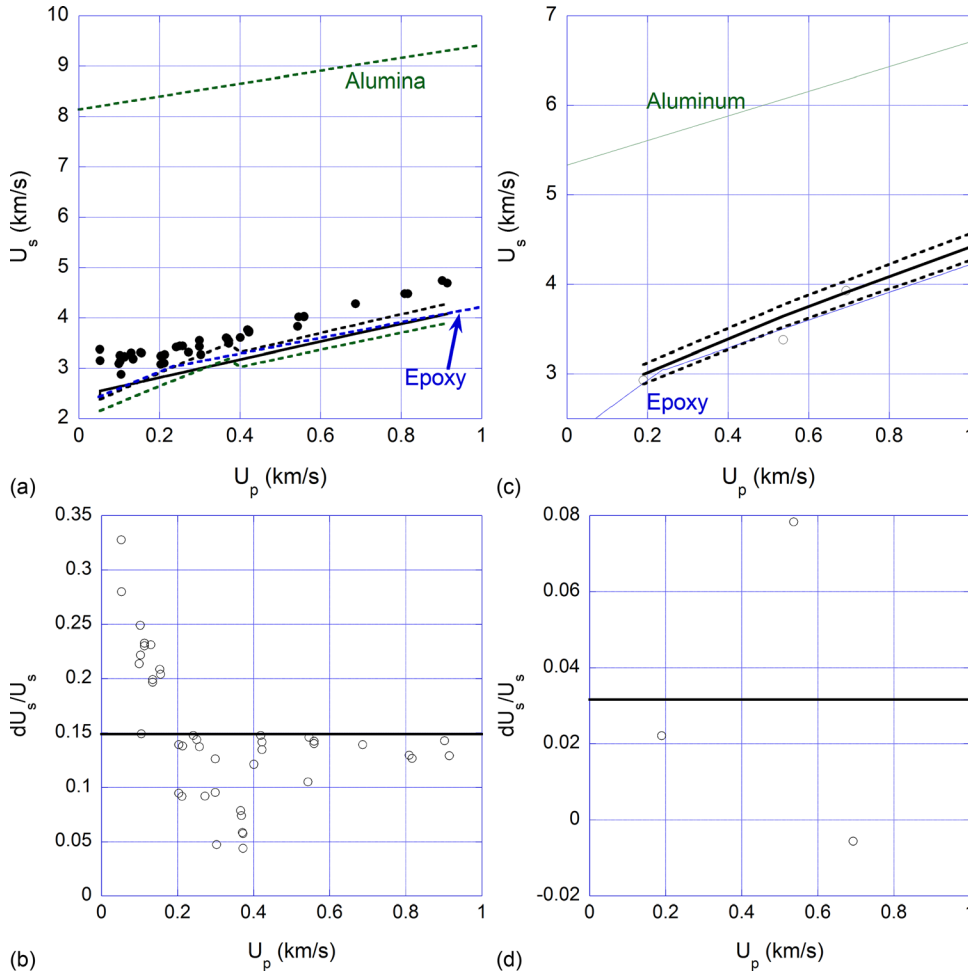
FIG. 4. (a) Particle velocity vs shock velocity and (b) dU_s/U_s for Al_2O_3-57 vol % epoxy and (c) particle velocity vs shock velocity and (d) dU_s/U_s for Al-55 vol % epoxy experimental data compared with mixture model calculation. The dashed lines on either side of the solid line in (a) indicated the error bars for the model calculation.

phase change in iron; however, the agreement for this three component system is as good as that for the uranium-rhodium composite.

2. Epoxy-Al-Fe₂O₃ and epoxy-Al-MnO₂

Two multi-component epoxy-based composites have sufficient experimental data available in the literature, epoxy-Al-Fe$_2$O$_3$ (Ref. 35) and epoxy-Al-MnO$_2$.[36] The input data for epoxy and aluminum have been discussed in the previous section. The equation of state for MnO$_2$ was determined from that for pyrolusite, as presented in Ref. 22. All of the input data for the multi-phase composites is given in Table V. The equations of state for Fe$_2$O$_3$ and MnO$_2$ are presented graphically in Fig. 6 with their associated variation in shock wave speed. For both materials, epoxy was chosen as material "1," or the reference material, for Eqs. (7)–(15). However, the model is insensitive to the choice of the reference material, and simulations of the epoxy-Al-Fe$_2$O$_3$ system

TABLE IV. Constituent and composite parameters for 304 stainless steel and its constituents.

Material	ρ_0 (g/cm^3)	C_0 (km/s)	S	ϕ^0	Refs.
Fe	7.85	3.57	1.92	0.74	34
Ni	8.875	4.59	1.44	0.18	22
Cr	7.119	5.2	1.43	0.08	22
304 SS	7.89	4.56	1.50		22

were conducted with each constituent as the reference material with no change in the predicted mixture behavior.

The experimental data and predicted model for epoxy-Al-Fe$_2$O$_3$ is shown in Fig. 7(a) along with the linear fits to the equations of state for the constituents. It can be seen that there is reasonably good agreement between the model and the experimental data. The ~7% error, Fig. 7(b), may be primarily due to the scatter in the experimental data rather than systematic differences between the experiments and the simulation. The model and experimental data are very close to the equation of state for epoxy, which is most likely due to the high volume fraction of epoxy in this system.

The predicted model and the experimental data for epoxy-Al-MnO$_2$ are presented in Fig. 7(c). For this composite, the density from the mixture model did not have good agreement with the actual density measured for the composite. The MnO$_2$ powders displayed porosity in Ref. 10, so the initial density of the MnO$_2$ constituent was modified by matching the composite mixture density to the experimentally measured composite density. The adjusted density is shown in parentheses in Table IV. With the adjusted density the agreement between the experimental data and the model is approximately 13%, which is in line with the agreement with two-phase epoxy based composites.

The experimental data in this system lies above the epoxy equation of state, rather than around it as in the epoxy-Al-Fe$_2$O$_3$ system. This indicates that the decreased volume fraction of epoxy in this system is reducing the effect of the
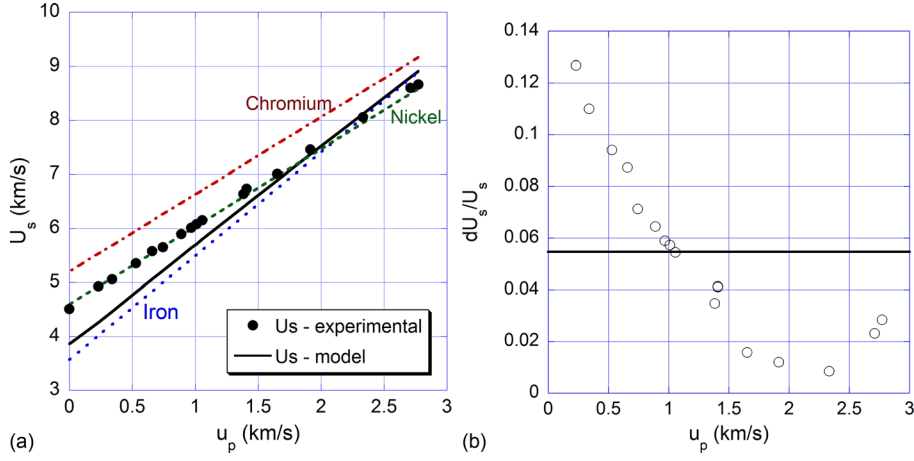
FIG. 5. (a) Particle velocity vs shock velocity and (b) dU_s/U_s for 304 stainless steel, experimental data (Ref. 20) compared with the mixture model calculation.
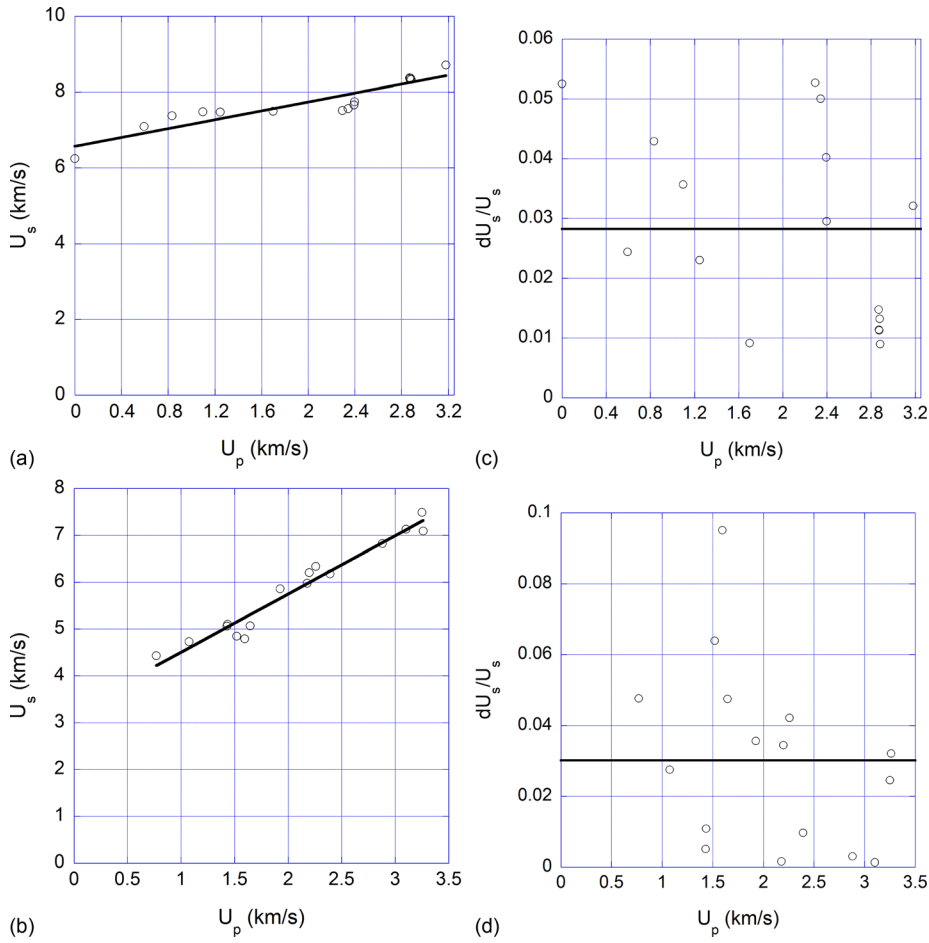

FIG. 6. Particle velocity vs shock velocity for (a) Fe_2O_3 and (b) MnO_2, where the circles are the experimental data from Ref. 20 and the solid line is a linear fit to these experimental data, and dU_s/U_s for (c) Fe_2O_3 and (d) MnO_2.

TABLE V. Constituent and composite parameters for epoxy-Al-Fe_2O_3 and epoxy-Al-MnO_2 materials.

Material	ρ_0 (g/cm^3)	C_0 (km/s)	S	ϕ^0_{epoxy}	$d\rho_0$	$d\phi^0$	dU_s	Refs.
Epoxy	1.134–1.194[a]				0.03		0.09	28–32
Aluminum	2.712	5.33	1.38		0.001		0.06	22
Iron oxide (Fe_2O_3)	5.00	6.24	1.39		0.01		0.21	22
Manganese dioxide (MnO_2)	5.03 (4.55)	3.261	1.24		0.01			22
Epoxy-Al-Fe_2O_3	2.366			0.60		0.01		35
Epoxy-Al-MnO_2	2.60	3.61[b]	1.47[b]	0.45	0.02	0.01		36

[a]Dependent on resin and curing agent.
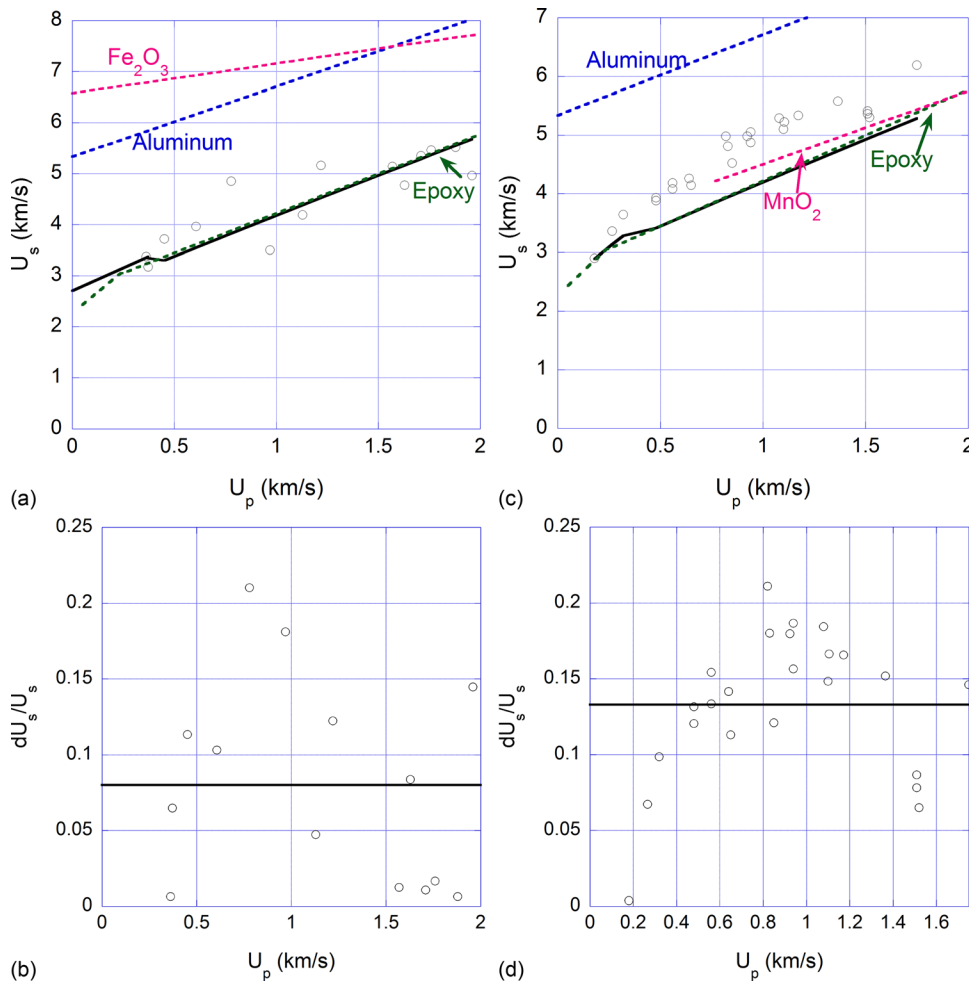[b]Linear fit $0.7 \leq u_p \leq 1.7$ km/s.

FIG. 7. (a) Particle velocity vs shock velocity and (b) dU_s/U_s for epoxy-Al-Fe$_2$O$_3$ and (c) particle velocity vs shock velocity and (d) dU_s/U_s for epoxy-Al-MnO$_2$ experimental (Refs. 30 and 31) data compared with the mixture model calculation. The dashed lines on either side of the solid line in (a) indicated the error bars for the model calculation.

epoxy binder on the composite behavior. The model does not reflect this same change in the influence of the epoxy binder. Increasing the aluminum volume fraction in the model to 0.40 (versus 0.24 actually in the composite), and decreasing the epoxy volume fraction by a comparable amount, results in a model that more accurately reflects the behavior of the composite. This may indicate that the volume fraction of the components varied in the samples or that the equation of state approximated for MnO$_2$ is not accurate.

IV. CONCLUSIONS

A general mixture model for determining the shock equation of state of composite materials is presented. The model is completely flexible allowing for multiple (>2) constituents in the composite. Additionally, error propagation analysis for the two component mixture model has been accomplished. For metallic composites, i.e., uranium-rhodium and 304 stainless steel, the average error between experiment and model is ∼5%. The prediction error for epoxy-based composites increases to ∼10%–15% based on the uncertainty in the epoxy equation of state, which dominates the material behavior due to its relatively large volume fraction. This mixture model allows for prediction of the equation of state of complex composite materials within 5%–15% of the experimental data, which is consistent with variations that are realized in meso-scale modeling of similar materials. The model can be implemented in MatLab and

run in minutes on a desktop computer, which may provide an advantage over the longer running meso-scale simulations, which also require significant computational set-up to be able to run. This mixture model tool may be used to predict experiments involving complex materials that have not been previously tested, allowing for confidence in experimental timing and other parameters.

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